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# *N*-Ethyl-2,2-dimethyl-*N*-(3-methylphenyl)propanamide

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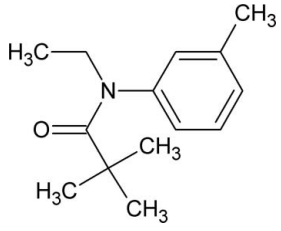
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.005 Å; disorder in main residue; $R$ factor = 0.057; $wR$ factor = 0.160; data-to-parameter ratio = 11.7.

In the title compound, $C_{14}H_{21}NO$, the conformation across the N—C(O) bond is *syn*-periplanar, the C—N—C—C torsion being −5.9 (5)°. The atoms of the ethyl group attached to the N atom are disordered over two sets of sites with occupancy ratios of 0.65 (2):0.35 (2) ($CH_2$) and 0.689 (14):0.311 (14) ($CH_3$)are linked by very weak C—H···O interactions forming $C(8)$ chains along [001]. C—H···$\pi$ interactions link the molecules along the *c*-axis direction.

## Related literature

For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the biological activity of amides, see: Manojkumar *et al.* (2013*a*,*b*). Amide groups can provide structural rigidity to molecules, see: Sreenivasa *et al.* (2013).




## Experimental

### Crystal data

$C_{14}H_{21}NO$
$M_r$ = 219.32
Monoclinic, $P2_1$
$a$ = 7.631 (4) Å
$b$ = 10.878 (7) Å
$c$ = 8.350 (3) Å
$\beta$ = 105.60 (2)°
$V$ = 667.6 (6) Å$^3$
$Z$ = 2
Cu $K\alpha$ radiation
$\mu$ = 0.52 mm$^{-1}$
$T$ = 294 K
0.22 × 0.20 × 0.16 mm

### Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.893, $T_{max}$ = 0.921
3786 measured reflections
2016 independent reflections
1883 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.160
$S$ = 1.06
2016 reflections
172 parameters
55 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

*Cg* is the centoid of the benzene ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···O$^{i}$ | 0.93 | 2.62 | 3.481 (2) | 153 |
| C14—H14$A$···$Cg^{ii}$ | 0.96 | 2.85 | 3.769 (8) | 161 |

Symmetry codes: (i) $x+1, y, z+1$; (ii) $x, y, z+1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5371).

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# supplementary materials

*Acta Cryst.* (2014). E**70**, o223 [doi:10.1107/S1600536814001718]

## *N*-Ethyl-2,2-dimethyl-*N*-(3-methylphenyl)propanamide

**B. S. Palakshamurthy, P. A. Suchetan, S Sreenivasa, N. K. Lokanath and T Madhu Chakrapani Rao**

### 1. Comment

Amides are very common in nature, formed easily and provides structural rigidity to the molecules (Sreenivasa *et al.* 2013). Amides show a broad spectrum of pharmacological properties, including antibacterial (Manojkumar *et al.* 2013*a*), anti-inflammatory, antioxidant, analgesic and antiviral activity (Manojkumar *et al.* 2013*b*). Keeping this in mind, the crystal structure of the title compound was determined.

### 2. Experimental

N-Ethyl-3-methylaniline (1.00g,7.4 mmol) was taken in dry dichloromethane (10 mL) and the solution was cooled to 0 $^{o}$C. To this reaction mixture 2,2-dimethylpropanoyl chloride (0.888 g, 7.4 mmol) in dichloromethane and triethylamine (1.49g, 1.48 mmol) were added slowly and the mixture was heated to 50$^{o}$C for 4 hours. Reaction was monitored by TLC. Reaction mixture was cooled and washed with 10% $NaHCO_3$ solution. The organic layer was separated, dried and concentrated to obtained crude product which was purified by column chromatography using petroleum ether: ethyl acetate (7:3) as eluent. Yellow prisms of the title compound were obtained from slow evapouration of the solution of the compound in petroleum ether: ethyl acetate (7:3).

### 3. Refinement

The H atoms were positioned with idealized geometry using a riding model with C-H = 0.93-0.96Å. All H atoms were refined with isotropic displacement parameters (set to 1.2-1.5 times of the Ueq of the parent atom). Flack parameter value (Flack, 1983) of 0.5 (5) was obtained in the final structure factor calculation, the presence of pseudosymmetry can lead to uncertainties about the correct space group, especially in the presence of twinning.

The C8 and C9 atoms of the ethyl group attached to N atom are disordered with site occupation factors of 0.65 (2):0.35 (2) and 0.689 (14):0.311 (14) respectively.

### Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

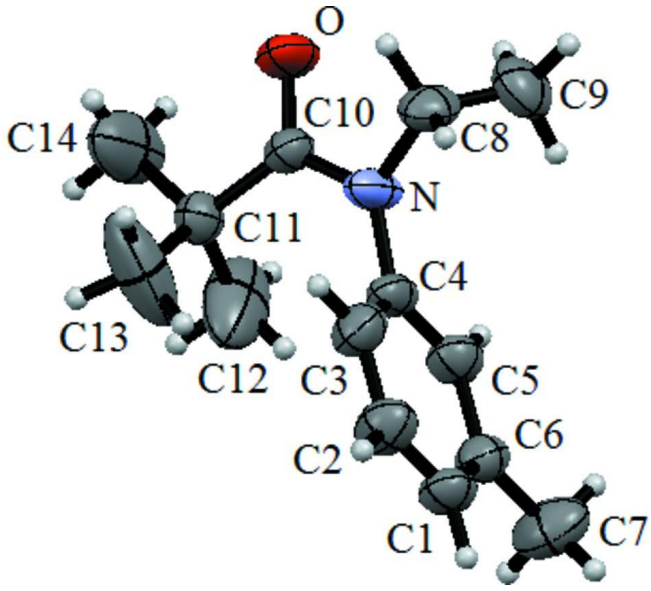


**Figure 1**

Molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level. Only the major components of the disordered atoms are shown.

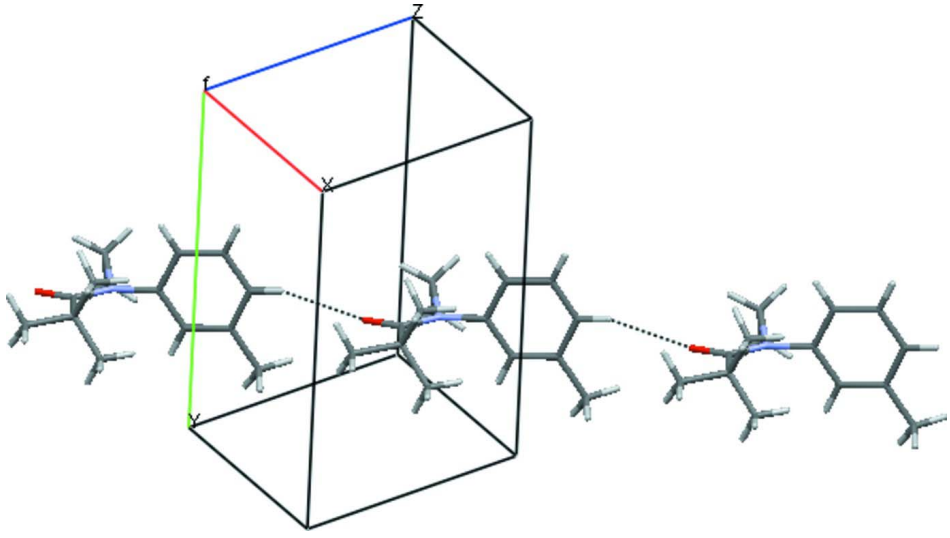


**Figure 2**

Molecular packing foming C(8) chains with hydrogen bonding shown as dashed lines.

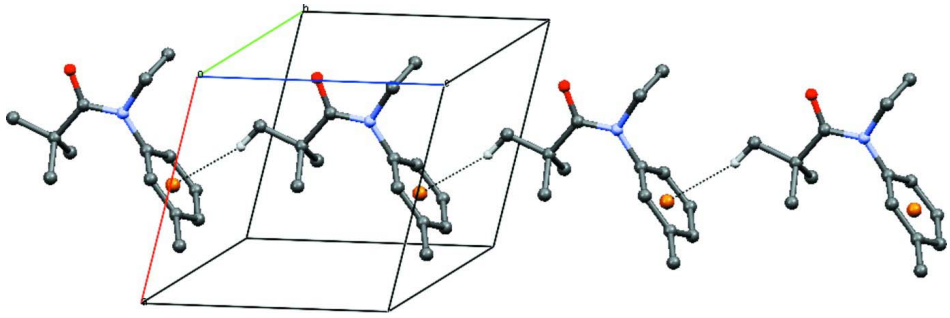

**Figure 3**

Stacking of molecules along *c* axis through C—H···*Cg* interactions. *Cg* is the centroid of the benzene ring. H-atoms not involved in H-bonding are ommitted for clarity.

### *N*-Ethyl-2,2-dimethyl-*N*-(3-methylphenyl)propanamide

*Crystal data*

$C_{14}H_{21}NO$
$M_r = 219.32$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 7.631$ (4) Å
$b = 10.878$ (7) Å
$c = 8.350$ (3) Å
$\beta = 105.60$ (2)°
$V = 667.6$ (6) Å$^3$
$Z = 2$
$F(000) = 240$
Prism
$D_x = 1.091$ Mg m$^{-3}$
Melting point: 492 K
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 172 reflections
$\theta = 5.5$–$65.5°$
$\mu = 0.52$ mm$^{-1}$
$T = 294$ K
Prism, yellow
0.22 × 0.20 × 0.16 mm

*Data collection*

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.893$, $T_{max} = 0.921$
3786 measured reflections
2016 independent reflections
1883 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 65.5°$, $\theta_{min} = 5.5°$
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 12$
$l = -9 \rightarrow 9$
1012 standard reflections every 2 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.160$
$S = 1.06$
2016 reflections
172 parameters
55 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.093P)^2 + 0.1495P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.16$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.018 (4)

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O | 0.2284 (2) | 0.7636 (3) | 0.6964 (2) | 0.0725 (7) | |
| N | 0.4145 (3) | 0.7530 (3) | 0.9461 (2) | 0.0670 (8) | |
| C11 | 0.5373 (3) | 0.7418 (3) | 0.6942 (3) | 0.0489 (6) | |
| C6 | 0.8300 (4) | 0.8185 (3) | 1.2843 (3) | 0.0494 (6) | |
| C10 | 0.3855 (3) | 0.7522 (3) | 0.7806 (3) | 0.0452 (6) | |
| C4 | 0.5820 (3) | 0.7342 (3) | 1.0730 (3) | 0.0487 (7) | |
| C5 | 0.6765 (4) | 0.8340 (3) | 1.1519 (3) | 0.0520 (7) | |
| H5 | 0.6374 | 0.9128 | 1.1164 | 0.062* | |
| C3 | 0.6371 (4) | 0.6191 (3) | 1.1298 (3) | 0.0586 (8) | |
| H3 | 0.5716 | 0.5510 | 1.0789 | 0.070* | |
| C2 | 0.7875 (4) | 0.6028 (3) | 1.2607 (4) | 0.0602 (8) | |
| H2 | 0.8249 | 0.5239 | 1.2975 | 0.072* | |
| C1 | 0.8829 (4) | 0.7029 (3) | 1.3376 (3) | 0.0520 (7) | |
| H1 | 0.9848 | 0.6916 | 1.4271 | 0.062* | |
| C7 | 0.9325 (5) | 0.9283 (4) | 1.3690 (5) | 0.0834 (11) | |
| H7A | 0.9820 | 0.9109 | 1.4851 | 0.125* | |
| H7B | 0.8515 | 0.9974 | 1.3563 | 0.125* | |
| H7C | 1.0295 | 0.9472 | 1.3200 | 0.125* | |
| C14 | 0.4518 (6) | 0.7552 (8) | 0.5111 (5) | 0.129 (2) | |
| H14A | 0.5454 | 0.7608 | 0.4542 | 0.193* | |
| H14B | 0.3787 | 0.8283 | 0.4908 | 0.193* | |
| H14C | 0.3766 | 0.6849 | 0.4710 | 0.193* | |
| C13 | 0.6307 (11) | 0.6209 (5) | 0.7262 (9) | 0.136 (3) | |
| H13A | 0.5417 | 0.5564 | 0.7079 | 0.205* | |
| H13B | 0.7044 | 0.6178 | 0.8392 | 0.205* | |
| H13C | 0.7066 | 0.6103 | 0.6523 | 0.205* | |
| C12 | 0.6785 (8) | 0.8393 (6) | 0.7487 (7) | 0.135 (3) | |
| H12A | 0.7324 | 0.8325 | 0.8663 | 0.202* | |
| H12B | 0.6230 | 0.9187 | 0.7237 | 0.202* | |
| H12C | 0.7708 | 0.8293 | 0.6910 | 0.202* | |
| C8A | 0.2598 (9) | 0.7879 (9) | 1.0135 (7) | 0.052 (2) | 0.65 (2) |
| H8A1 | 0.1744 | 0.8395 | 0.9348 | 0.063* | 0.65 (2) |
| H8A2 | 0.3035 | 0.8329 | 1.1169 | 0.063* | 0.65 (2) |
| C8B | 0.2459 (15) | 0.7104 (19) | 1.0046 (14) | 0.059 (4) | 0.35 (2) |
| H8B1 | 0.1529 | 0.6742 | 0.9142 | 0.070* | 0.35 (2) |
| H8B2 | 0.2801 | 0.6522 | 1.0958 | 0.070* | 0.35 (2) |
| C9A | 0.1691 (10) | 0.6700 (7) | 1.0428 (8) | 0.087 (2) | 0.689 (14) |

| | | | | | |
|---|---|---|---|---|---|
| H9A1 | 0.1289 | 0.6256 | 0.9400 | 0.131* | 0.689 (14) |
| H9A2 | 0.0664 | 0.6887 | 1.0843 | 0.131* | 0.689 (14) |
| H9A3 | 0.2542 | 0.6207 | 1.1226 | 0.131* | 0.689 (14) |
| C9B | 0.1877 (19) | 0.8243 (14) | 1.0567 (15) | 0.071 (4) | 0.311 (14) |
| H9B1 | 0.2883 | 0.8636 | 1.1337 | 0.107* | 0.311 (14) |
| H9B2 | 0.0925 | 0.8096 | 1.1096 | 0.107* | 0.311 (14) |
| H9B3 | 0.1429 | 0.8765 | 0.9617 | 0.107* | 0.311 (14) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O | 0.0395 (10) | 0.130 (2) | 0.0405 (9) | 0.0096 (12) | −0.0029 (8) | −0.0003 (11) |
| N | 0.0294 (10) | 0.136 (2) | 0.0338 (10) | 0.0065 (14) | 0.0055 (8) | 0.0032 (14) |
| C11 | 0.0481 (13) | 0.0608 (15) | 0.0394 (12) | 0.0028 (13) | 0.0147 (10) | 0.0013 (11) |
| C6 | 0.0429 (14) | 0.0613 (17) | 0.0417 (12) | −0.0053 (13) | 0.0072 (10) | 0.0004 (12) |
| C10 | 0.0375 (12) | 0.0603 (14) | 0.0343 (11) | −0.0002 (12) | 0.0038 (9) | −0.0004 (11) |
| C4 | 0.0336 (12) | 0.0806 (19) | 0.0298 (10) | 0.0034 (13) | 0.0051 (9) | 0.0036 (12) |
| C5 | 0.0456 (15) | 0.0645 (17) | 0.0427 (13) | 0.0073 (13) | 0.0063 (11) | 0.0077 (12) |
| C3 | 0.0559 (17) | 0.0689 (19) | 0.0469 (15) | −0.0075 (15) | 0.0067 (13) | −0.0085 (13) |
| C2 | 0.0631 (18) | 0.0565 (17) | 0.0542 (15) | 0.0061 (14) | 0.0040 (14) | 0.0069 (13) |
| C1 | 0.0417 (15) | 0.0677 (18) | 0.0404 (12) | 0.0050 (13) | 0.0003 (11) | 0.0069 (12) |
| C7 | 0.079 (2) | 0.073 (2) | 0.083 (3) | −0.0182 (19) | −0.0049 (19) | −0.0069 (18) |
| C14 | 0.086 (3) | 0.254 (7) | 0.0529 (18) | 0.027 (4) | 0.0323 (19) | 0.021 (3) |
| C13 | 0.189 (6) | 0.118 (4) | 0.150 (5) | 0.083 (4) | 0.126 (5) | 0.052 (3) |
| C12 | 0.134 (4) | 0.178 (5) | 0.125 (4) | −0.087 (4) | 0.091 (4) | −0.062 (4) |
| C8A | 0.038 (3) | 0.075 (5) | 0.045 (2) | 0.006 (3) | 0.0115 (19) | −0.008 (3) |
| C8B | 0.037 (5) | 0.083 (10) | 0.054 (5) | −0.014 (6) | 0.009 (4) | 0.001 (5) |
| C9A | 0.066 (4) | 0.110 (5) | 0.101 (4) | −0.013 (3) | 0.049 (3) | 0.001 (4) |
| C9B | 0.057 (7) | 0.095 (8) | 0.073 (7) | 0.006 (6) | 0.035 (5) | 0.003 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O—C10 | 1.222 (3) | C7—H7C | 0.9600 |
| N—C10 | 1.339 (3) | C14—H14A | 0.9600 |
| N—C4 | 1.439 (3) | C14—H14B | 0.9600 |
| N—C8A | 1.488 (7) | C14—H14C | 0.9600 |
| N—C8B | 1.564 (12) | C13—H13A | 0.9600 |
| C11—C13 | 1.486 (5) | C13—H13B | 0.9600 |
| C11—C12 | 1.493 (5) | C13—H13C | 0.9600 |
| C11—C14 | 1.499 (5) | C12—H12A | 0.9600 |
| C11—C10 | 1.525 (3) | C12—H12B | 0.9600 |
| C6—C1 | 1.359 (4) | C12—H12C | 0.9600 |
| C6—C5 | 1.388 (4) | C8A—C9A | 1.508 (13) |
| C6—C7 | 1.497 (5) | C8A—H8A1 | 0.9700 |
| C4—C3 | 1.364 (4) | C8A—H8A2 | 0.9700 |
| C4—C5 | 1.370 (4) | C8B—C9B | 1.42 (3) |
| C5—H5 | 0.9300 | C8B—H8B1 | 0.9700 |
| C3—C2 | 1.367 (4) | C8B—H8B2 | 0.9700 |
| C3—H3 | 0.9300 | C9A—H9A1 | 0.9600 |

| | | | |
|---|---|---|---|
| C2—C1 | 1.370 (4) | C9A—H9A2 | 0.9600 |
| C2—H2 | 0.9300 | C9A—H9A3 | 0.9600 |
| C1—H1 | 0.9300 | C9B—H9B1 | 0.9600 |
| C7—H7A | 0.9600 | C9B—H9B2 | 0.9600 |
| C7—H7B | 0.9600 | C9B—H9B3 | 0.9600 |

| | | | |
|---|---|---|---|
| C10—N—C4 | 128.83 (19) | H7B—C7—H7C | 109.5 |
| C10—N—C8A | 117.7 (3) | C11—C14—H14A | 109.5 |
| C4—N—C8A | 113.3 (2) | C11—C14—H14B | 109.5 |
| C10—N—C8B | 113.5 (5) | H14A—C14—H14B | 109.5 |
| C4—N—C8B | 111.7 (4) | C11—C14—H14C | 109.5 |
| C13—C11—C12 | 107.6 (5) | H14A—C14—H14C | 109.5 |
| C13—C11—C14 | 109.0 (4) | H14B—C14—H14C | 109.5 |
| C12—C11—C14 | 108.8 (4) | C11—C13—H13A | 109.5 |
| C13—C11—C10 | 111.7 (3) | C11—C13—H13B | 109.5 |
| C12—C11—C10 | 112.4 (3) | H13A—C13—H13B | 109.5 |
| C14—C11—C10 | 107.3 (2) | C11—C13—H13C | 109.5 |
| C1—C6—C5 | 119.1 (3) | H13A—C13—H13C | 109.5 |
| C1—C6—C7 | 120.8 (3) | H13B—C13—H13C | 109.5 |
| C5—C6—C7 | 120.1 (3) | C11—C12—H12A | 109.5 |
| O—C10—N | 117.2 (2) | C11—C12—H12B | 109.5 |
| O—C10—C11 | 119.2 (2) | H12A—C12—H12B | 109.5 |
| N—C10—C11 | 123.6 (2) | C11—C12—H12C | 109.5 |
| C3—C4—C5 | 119.1 (2) | H12A—C12—H12C | 109.5 |
| C3—C4—N | 121.1 (3) | H12B—C12—H12C | 109.5 |
| C5—C4—N | 119.3 (3) | N—C8A—C9A | 106.8 (6) |
| C4—C5—C6 | 120.6 (3) | N—C8A—H8A1 | 110.4 |
| C4—C5—H5 | 119.7 | C9A—C8A—H8A1 | 110.4 |
| C6—C5—H5 | 119.7 | N—C8A—H8A2 | 110.4 |
| C4—C3—C2 | 120.7 (3) | C9A—C8A—H8A2 | 110.4 |
| C4—C3—H3 | 119.6 | H8A1—C8A—H8A2 | 108.6 |
| C2—C3—H3 | 119.6 | C9B—C8B—N | 100.9 (13) |
| C3—C2—C1 | 119.9 (3) | C9B—C8B—H8B1 | 111.6 |
| C3—C2—H2 | 120.1 | N—C8B—H8B1 | 111.6 |
| C1—C2—H2 | 120.1 | C9B—C8B—H8B2 | 111.6 |
| C6—C1—C2 | 120.6 (2) | N—C8B—H8B2 | 111.6 |
| C6—C1—H1 | 119.7 | H8B1—C8B—H8B2 | 109.4 |
| C2—C1—H1 | 119.7 | C8A—C9A—H9A1 | 109.5 |
| C6—C7—H7A | 109.5 | C8A—C9A—H9A2 | 109.5 |
| C6—C7—H7B | 109.5 | H9A1—C9A—H9A2 | 109.5 |
| H7A—C7—H7B | 109.5 | C8A—C9A—H9A3 | 109.5 |
| C6—C7—H7C | 109.5 | H9A1—C9A—H9A3 | 109.5 |
| H7A—C7—H7C | 109.5 | H9A2—C9A—H9A3 | 109.5 |

| | | | |
|---|---|---|---|
| C4—N—C10—O | 175.9 (3) | C8B—N—C4—C5 | −109.8 (9) |
| C8A—N—C10—O | −9.8 (6) | C3—C4—C5—C6 | 2.2 (4) |
| C8B—N—C10—O | 25.7 (9) | N—C4—C5—C6 | 174.5 (2) |
| C4—N—C10—C11 | −5.9 (5) | C1—C6—C5—C4 | −1.7 (4) |
| C8A—N—C10—C11 | 168.3 (5) | C7—C6—C5—C4 | 179.8 (3) |

| | | | |
|---|---|---|---|
| C8B—N—C10—C11 | −156.1 (9) | C5—C4—C3—C2 | −1.8 (4) |
| C13—C11—C10—O | −116.5 (5) | N—C4—C3—C2 | −174.0 (3) |
| C12—C11—C10—O | 122.5 (4) | C4—C3—C2—C1 | 0.9 (5) |
| C14—C11—C10—O | 2.9 (5) | C5—C6—C1—C2 | 0.8 (4) |
| C13—C11—C10—N | 65.3 (5) | C7—C6—C1—C2 | 179.3 (3) |
| C12—C11—C10—N | −55.7 (5) | C3—C2—C1—C6 | −0.4 (4) |
| C14—C11—C10—N | −175.2 (4) | C10—N—C8A—C9A | 94.8 (5) |
| C10—N—C4—C3 | −88.2 (4) | C4—N—C8A—C9A | −90.0 (5) |
| C8A—N—C4—C3 | 97.3 (5) | C8B—N—C8A—C9A | 4.1 (8) |
| C8B—N—C4—C3 | 62.4 (9) | C10—N—C8B—C9B | −107.2 (7) |
| C10—N—C4—C5 | 99.6 (4) | C4—N—C8B—C9B | 97.4 (8) |
| C8A—N—C4—C5 | −74.9 (5) | C8A—N—C8B—C9B | −2.2 (6) |

*Hydrogen-bond geometry (Å, º)*

Cg is the centoid of the benzene ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···O$^{i}$ | 0.93 | 2.62 | 3.481 (2) | 153 |
| C14—H14*A*···*Cg*$^{ii}$ | 0.96 | 2.85 | 3.769 (8) | 161 |

Symmetry codes: (i) *x*+1, *y*, *z*+1; (ii) *x*, *y*, *z*+1.